

Atomic orbital analysis of NbSe₂ valence band

by display-type analyzer (DIANA)

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1. Introduction

Layered transition-metal dicalcogenides (TMDC) have quasi two-dimensional system and their transport properties extend from metal and semiconductor to insulator. Some of them show charge-density wave and superconducting phase transitions. NbSe₂ is one of the typical materials that show charge-density waves (CDW), and serves an appropriate playground for the study of CDW mechanism [1][2]. Therefore the study of the electronic structure of NbSe₂ is very important not only to understand the properties of NbSe₂, but also to clarify the CDW mechanism.

Angle-resolved photoelectron spectroscopy (ARPES) is a useful method to measure the topology of Fermi surface and the gaps associated with phase transitions of CDW and superconductivity. To clarify the mechanism of these fascinating properties, it is indispensable to study the topology of Fermi surface and analyses of atomic orbitals which compose the bands near the Fermi level. Nevertheless, experimental and theoretical studies of atomic orbitals of NbSe₂ are still lacking.

To obtain experimental information of the atomic orbitals near Fermi level of NbSe₂, we have measured photoelectron angular distribution (PEAD) patterns with various sample azimuthal orientations from Fermi level of NbSe₂ by display-type analyzer (DIANA).

2. ARPES and DIANA

Angle-resolved photoelectron spectroscopy (ARPES) is a method to measure band

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dispersions directly. When light is focused onto the surface of a material, the photon is absorbed and a photoelectron is excited. The binding energy and momentum of electrons in initial state can be derived from the kinetic energy and emission angle of photoelectrons. Though photoelectrons escape into vacuum in wide solid angle, conventional analyzers detect photoelectrons in narrow solid angle. In order to measure the photoelectron intensity distribution in all solid angle, it takes much time. In fact, three-dimensional mapping of Fermi surface is unrealistic.

By using DIANA, one can measure photoelectrons in wide solid angle at once. The obtained PEAD pattern has no distortion. As a result, DIANA saves a lot of time to measure photoelectrons intensity distributions. Furthermore using DIANA with polarized and energy tunable light source from synchrotron radiation, one can measure three-dimensional Fermi surface and analyze atomic orbitals which compose bands.

3. Experiment

The experiment was performed at beamline 7 of Ritsumeikan SR center. The clean surface was prepared by cleaving the samples in ultrahigh vacuum. Fig.1 shows the crystal structure of 2H-NbSe₂. The energy band and crystal structure of 2H-NbSe₂ has six-fold symmetry. In this crystal structure, a Nb atom layer is sandwiched between two Se layers. The sandwich layers are coupled only by weak van der Waals forces. Therefore if it is cleaved, the inert surface of Se layer will appear.

The incident photons were linearly polarized and the photon energy at this experiment was set to 45 eV. PEAD patterns with various sample azimuthal orientations from Fermi level were taken with DIANA equipped at beamline 7.

The energy resolution($\Delta E/E$) was 1% and angel resolution was 1° . Typical acquisition time for one PEAD was 10 min.

4. Result and discussion

PEAD pattern is determined by the transition matrix from an atomic orbital considering the electric vector of the incident light [3]. Fig. 2 shows calculated PEAD patterns from various *d*-orbitals. PEAD pattern of each *d*-orbital changes, if azimuthal angle ϕ varies.

Fig. 3 shows PEAD patterns from Fermi level, with sample azimuthal angles of 0° and 30° . The band dispersion around Γ point was split to two parts because of the transition matrix. Theoretical studies pointed out that the band at Fermi level is mainly composed of *d*-orbital. In spite of azimuthal rotation of the sample, PEAD patterns around Γ point in Fig. 3. (a), (b) didn't change. This suggests that the atomic orbital which composes the band around Γ point is symmetric around the light axis. As a result, we obtained the experimental information that the atomic orbit which composes the band around Γ point is mainly d_{z^2} .

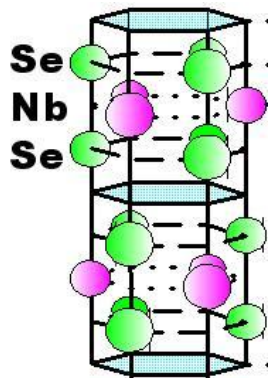


Fig. 1. Crystal structure of 2HNbSe₂

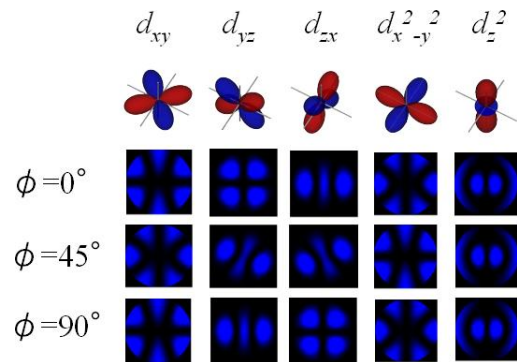


Fig. 2. Calculated PEAD patterns from various d-orbitals[3]

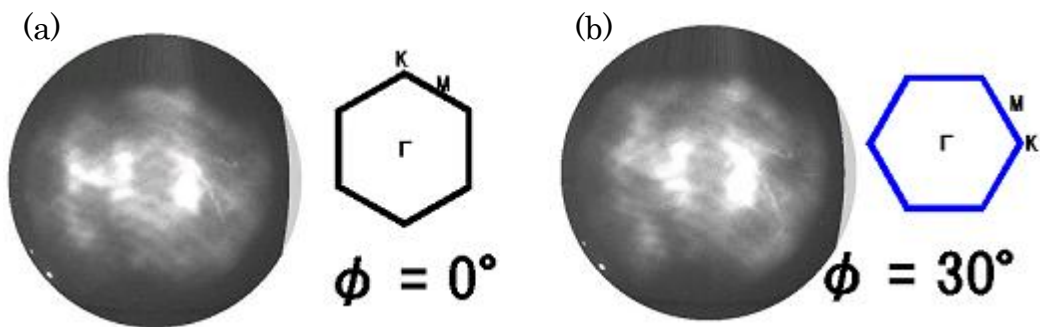


Fig. 3. PEAD patterns from Fermi level of 2H-NbSe₂ with azimuthal angles of (a) 0° and (b) 30° .

References

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